

CURRICULUM VITAE

Yorley Andrea Duarte

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Office Address: Centro de Bioinformática y Biología Integrativa República 330 piso 1.
Universidad Andrés Bello
Edificio de Investigación Santiago Centro
Santiago, 8320000, Chile

Phone: 56-2-2770 3612
e-mail1: yorley.duarte@unab.cl
e-mail2: yorandre53@gmail.com

Education:

2011-2015 Universidad de Talca Ph.D. in Applied Sciences
2006-2009 Universidad Nacional de Colombia, MsC. Chemical Science
2000-2005 Universidad Pedagógica y Tecnológica Colombia, Food Chemist

Professional and other Positions:

2020-present Assistant Professor, Center for Bioinformatics and Integrative Biology (CBIB), Faculty of Live Sciences, Universidad Andrés Bello.
2015-2020 Postdoctoral researcher, CBIB, Faculty of Live Sciences, Universidad Andrés Bello.
2018-2020 Postdoctoral researcher in the Fondef ID18I10235, CIBIB, Faculty of Live Sciences, Universidad Andrés Bello.
2015-2017 Postdoctoral researcher in the CORFO project 14IDL2-30195, CIBIB, Faculty of Live Sciences, Universidad Andrés Bello.
2010-2015 Graduate Student, laboratory of Medical chemistry, Instituto de Química de Recursos Naturales (IQRN) and Center for Bioinformatics and Molecular Simulation (CBSM), Universidad de Talca, Chile.
2010 Occasional Professor, Chemistry Department, Faculty of Basic Sciences, Universidad del Atlántico, Colombia.
2007-2009 Master Student, Heterocycles Laboratory, Chemistry Department, Faculty of Sciences, Universidad Nacional de Colombia.
2008- 2009 Teaching assistant student, Food Science and Technology Specialization, Faculty of Agricultural Sciences, Universidad Nacional de Colombia.

Major Research Interests:

Our research focuses on the search and rational design of new molecules that inhibit or modulate various membrane or cytosolic proteins' function, using drug discovery strategies based on in silico studies and medicinal chemistry methods. Simultaneously, we have the tools and knowledge of conventional and combinatorial Chemical Synthesis to obtain and synthetically modify leading molecules to improve their affinity and biological activity against a particular target. Using nanotechnology and chemical synthesis strategies, we develop new controlled drug release systems, through dendrimers functionalization and the rationalization of the components of liposomes and biopolymers, controlling the peripheral chemical groups, to improve the affinity with the drug of interest and the target to which it will be directed.

At present, we center our interest in discovering, design, and synthesizing through a combination of experimental and in silico drug-discovery pipelines a set of new molecules that block and inhibit inx2 GJ channels function with low cytotoxicity. The innexin2 channel is associated with the *Caligus rogercresseyi* parasite, which is the most significant sea lice species affecting the country's salmon industry. Through virtual screening, we search for new Innexin1 inhibitors, channel involved in the *Anopheles gambiae* mosquito function, to contribute the knowledge of new targets and inhibitors related to Malaria disease.

Research Grants:

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| 2020-2023 | Innexin2 hemichannels of <i>caligus rogercresseyi</i> as a new target to design antiparasitic agents through in-silico structure-based drug discovery, chemical synthesis and biological assays FONDECYT 11201113. Chilean Gov. Principal Investigator. |
| 2021-2025 | Newly piperazinone derivatives with antithrombotic and anti-inflammatory properties: environmentally-friendly synthesis, characterization, and biological evaluation. FONDECYT 1210763. Chilean Gov. co-Investigator. |
| 2020-2023 | Hybrids of Tetrahydroquinolines as Multi-Target drugs: Design, Synthesis, characterization and biological activity. FONDECYT 1200531. Chilean Gov. co-Investigator. |
| 2019-2023 | Diverse cell types present pannexin1-based gap junction channels with distinct regulatory, functional and pharmacological properties. FONDECYT 1191329. Chilean Gov. co-Investigator. |
| 2020-2021 | Developing in a Nanobubble Technology for Blast Dust Control Systems. CORFO project 11CVC-118661. Associate Investigator. |
| 2019-2021 | Synthetic functionalization and pharmacological evaluation of mitochondria-targeted dendrimer . Nucleo UNAB DI-01-19/N. Institutional grant. Associate Investigator. |
| 2015-2019 | Innexin1 hemichannels of <i>Plasmodium falciparum</i> as a new target to design antimalaric agents through in-silico structure-based drug discovery and chemical synthesis. Laureate International grant. Associate Investigator. |

Original publications:

- 1-** Rivera A., Duarte Y., González-Salas D., Ríos-Motta J., Zaragoza G. X-ray and Hydrogen-bonding Properties of 1-((1H-benzo-triazol-1-yl)methyl)naphthalen-2-ol. *Molecules*. 2009, 14, 1234-1244.
- 2-** Duarte Y., Gutiérrez M., Astudillo L., Brito I., Cárdenas A., Bolteand M., López-Rodríguez M. Crystal structure of 1,3-bis(6-methoxyquinolin-2-yl)benzene, C₂₆H₂₀N₂O₂. *Z. Kristallogr.* 228, 2013, 371-72.
- 3-** Duarte Y, Gutiérrez M, Astudillo L, Alzate-Morales J, Valdés N. Synthesis of bistetrahydroquinolines as potential anticholinesterasic agents by double Diels-Alder reactions. *Molecules*. 2013, 18, 12951-65.
- 4-** Duarte Y, Dueñas F, Gutiérrez M. Tetrahydroquinolines and Isoxazoles: Nitroge heterocycles as potential antibacterial agents. *JOCPR*, 2015, 7(3):294-299.
- 5-** Fonseca A., Matos M., Reis J., Duarte Y., Gutiérrez M., Santana L., Uriarte E., and Borges F. Exploring coumarin potentialities: development of new MAO-B inhibitors based on the 6-methyl-3-carboxamidocoumarin scaffold. *RSC Adv.*, 2016, 6, 49764-49768.
- 6-** Duarte Y., Fonseca A., Gutiérrez M., Adasme-Carreño F., Muñoz-Gutierrez C., Alzate-Morales J., Santana L., Uriarte E., Álvarez R., Matos MJ. Novel Coumarin-Quinoline Hybrids: Design of Multitarget Compounds for Alzheimer's Disease. *ChemistrySelect* 2019, 4, 551 –558.
- 7-** Duarte Y., Gutiérrez M., Álvarez R., Alzate-Morales J., Soto-Delgado J. Experimental and theoretical approaches in the study of phenanthroline-tetrahydroquinolines for Alzheimer's disease. *Chemistryopen*. 2019, 8, 627–636.
- 8-** Santana-Romo F., Lagos C. F., Duarte Y., Castillo F., Moglie Y., Maestro M.A., Charbe N., Zacconi F.C.. Innovative Three-Step Microwave-Promoted Synthesis of N-Propargyl tetrahydroquinoline and 1,2,3-Triazole Derivatives as a Potential Factor Xa (FXa) Inhibitors: Drug Design, Synthesis, and Biological Evaluation. *Molecules* 2020, 25, 491.
- 9-** Lozano-Cruz T., Alcarraz-Vizán G., de la Mata F. J., de Pablo S., Ortega P., Duarte Y, Bravo-Moraga F., D. González-Nilo F., Novials A., Gómez R. Cationic carbosilane dendritic systems as promising anti-amyloid agents in type 2 diabetes. *Chemistry*. 2020;26(34):7609-7621.
- 10-** Ulzurrun E, Duarte Y, Perez-Wohlfeil E, Gonzalez-Nilo F, Trelles O. PLIDflow: an open-source workflow for the online analysis of protein-ligand docking using galaxy. *Bioinformatics*. 2020;36(14):4203-4205.
- 11-** Duarte Y., Cáceres J., Sepúlveda R. V., Arriagada D., Olivares P., Díaz-Franulic I., Stehberg J., González-Nilo F.. Novel TRPV1 Channel Agonists with Faster and More Potent Analgesic Properties Than Capsaicin. *Front. Pharmacol.*, 2020, 14.
- 12-** Doñate-Macian P., Duarte Y., Rubio-Moscardo F., Pérez-Vilaró G., Canan J., Díez J., González-Nilo F., Valverde M.A. Structural determinants of TRPV4 inhibition and identification of new antagonists with antiviral activity. *Br J Pharmacol*. 2020; 1– 16.
- 13-** López X., Escamilla R., Fernandez P., Duarte Y., González-Nilo F., Palacios-Prado N., Martinez A., Sáez J.C. Stretch-induced activation of pannexin 1 channels can be prevented by PKA- dependent phosphorylation. *IJMS* 2020, 2;21(23):9180.
- 14-** Duarte, Y.; Rojas, M.; Canan, J.; Pérez, E.G.; González-Nilo, F.; García-Colunga, J. Different Classes of Antidepressants Inhibit the Rat $\alpha 7$ Nicotinic Acetylcholine Receptor by

Interacting within the Ion Channel: A Functional and Structural Study. *Molecules* 2021, 26, 998.

Conference papers:

- 1-** Duarte, Y.; Arevalo, B.; Martinez, G.; Matus, F.; Poblete, T.; Gutierrez, M.; Amigo, J.; Vallejos, G.; Astudillo, L. Nitrogen Heterocycles as Potential Antibacterial Agents. In Proceedings of the 17th Int. Electron. Conf. Synth. Org. Chem., 1–30 November 2013; Sciforum Electronic Conference Series, Vol. 17, 2013, a035; doi:10.3390/ecsoc-17-a035.
- 2-** Fonseca, A.; Matos, M.; Duarte, Y.; Borges, F.; Santana, L.; Uriarte, E.; Gutiérrez, M.; Astudillo, L. Synthesis and Study of a Selected Series of Amides with the Coumarin Scaffold for the Treatment of Alzheimer's Disease. In Proceedings of the 17th Int. Electron. Conf. Synth. Org. Chem., 1–30 November 2013; Sciforum Electronic Conference Series, Vol. 17, 2013, b007; doi:10.3390/ecsoc-17-b007.

Reviews:

- 1-** Duarte Y., Márquez-Miranda V., Miossec M., González-Nilo F. Integration of target discovery, drug discovery and drug delivery: A review on computational strategies. *WIREs Nanomed Nanobiotechnol.* 2019; e1554.

Meeting abstracts:

- XXIX Congreso Latinoamericano de Química. Comportamiento del benzotriazol como grupo saliente en las reacciones de sustitución nucleofílica de N,N-bis(1H-benzotriazol-1-il-metil)-1,2-diaminobenceno con fenoles. Cartagena, Colombia 2010, 27.
- XVIII SINAQO. SINTESIS DE TETRAHIDROQUINOLINAS Y SU ACTIVIDAD BIOLÓGICA. Villa Carlos Paz, Argentina 2011, QO 73.
- XIX SINAQO. Synthesis of bistetrahydroquinolines as AchE inhibitor by double Diels-Alder reactions. Mar del Plata, Argentina 2013.
- III SEQT Summer School. NITROGEN HETEROCYCLES AS POTENTIAL AGENTS ANTI-ALZHEIMER, Madrid, España, 2013. 53.
- Workshop in Modern Approaches in Drug Discovery for Neglected Infectious diseases. Instituto Pasteur de Montevideo, Montevideo, Uruguay. Curso. 3-18/Nov-2014.
- 16th. BMOS. Experimental and Theoretical Study of phenanthroline-tetrahydroquinolines by Povarov Reaction. Búzios, Brazil, 2015. 100, 170.
- GTCbio's European Pharma Summit on November 16-17, 2017 in Berlin, Germany.
- X international Conference on Bioinformatics -SoIBio2019. The conference was held 28-30 October 2019 in Montevideo, Uruguay, at the Universidad de la República.
- XIX Jornadas Chilenas de Química. SINTESIS DE TETRAHIDROQUINOLINAS Y SU ACTIVIDAD BIOLÓGICA. Panimávida, Chile 2011, QO 198.
- ISCB-LA SoIBio EMBnet 2018 Joint Bioinformatics Conference. The conference was held 5-9 November 2018 in Vina Del Mar, Chile, at the Universidad Andres Bello

Thesis advice:

-Synthesis and study of biological activity of nitrogenous heterocycles analogous to quinolines. Michele Campos (Tecnología médica school). Universidad de Talca Chile 2014. Thesis co-advisor.

-Synthesis of coumarin-quinolinic hybrids as selective cholinesterase inhibitors. Rafael Latorre (Tecnología médica school). Universidad de Talca Chile 2014. Thesis co-advisor.

-Implementation of workflows with Schrödinger programs using KNIME for drug discovery. Juan Pablo Calderon. Universidad Andrés Bello Chile 2020 RESEARCH UNIT I

-Bibliographic review and Synthesis of PAMAM G3 coupled to caffeic and coumaric acid. Catalina Inostroza. Universidad Andrés Bello Chile 2020. Professional Practice Advisor.

Encapsulation of antioxidants in hybrid liposomes: formulation, characterization and pharmacological evaluation directed to mitochondria. Catalina Inostroza (Biochemistry school). Universidad Andrés Bello Chile. in progress. Thesis advisor